Homogenization of reaction-diffusion systems

Harsha Hutridurga

Joint work with Grégoire Allaire & Laurent Desvillettes

IIT Bombay

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REACTION-DIFFUSION SYSTEM: SETTING AND OBJECTIVE

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- These equations should model chemical species *reacting* with each other and *diffusing* in the spatial domain

SETTING AND OBJECTIVE

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- ♣ Species are involved in a reversible chemical reaction with rate function $\mathcal{R}_i(u)$ – net production/consumption of $\mathcal{A}_i$

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- ♣ Supplemented by initial and boundary data

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$$\alpha_1\mathcal{A}_1 + \cdots + \alpha_\ell\mathcal{A}_\ell \underset{\kappa_b}{\overset{\kappa_f}{\rightleftharpoons}} \beta_1\mathcal{A}_1 + \cdots + \beta_\ell\mathcal{A}_\ell$$

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- ♣ Take $(\alpha_1, \alpha_2, \alpha_3) = (1, 1, 0)$ and $(\beta_1, \beta_2, \beta_3) = (0, 0, 1)$

$$\mathcal{A}_1 + \mathcal{A}_2 \underset{\kappa\gamma}{\overset{\kappa}{\rightleftharpoons}} \mathcal{A}_3$$

$$\mathcal{R}_1(u) = \mathcal{R}_2(u) = -\kappa\big(u_1u_2 - \gamma u_3\big); \qquad \mathcal{R}_3(u) = \kappa\big(u_1u_2 - \gamma u_3\big)$$

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REVERSIBLE CHEMISTRY (CONTD.)

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♣ Take $(\alpha_1, \alpha_2, \alpha_3, \alpha_4) = (1, 0, 1, 0)$ and $(\beta_1, \beta_2, \beta_3, \beta_4) = (0, 1, 0, 1)$

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WE PRESENT COMPUTATIONS FOR THREE SPECIES SYSTEM

$$\mathcal{A}_1 + \mathcal{A}_2 \xrightleftharpoons[\kappa\gamma]{\kappa} \mathcal{A}_3$$

$$\begin{cases} \partial_t u_1^\varepsilon - \operatorname{div}\left(d_1(x)\mathbf{D}\left(\frac{x}{\varepsilon}\right)\nabla u_1^\varepsilon\right) = -\frac{\kappa}{\varepsilon^2}\left(u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon\right) \\ \partial_t u_2^\varepsilon - \operatorname{div}\left(d_2(x)\mathbf{D}\left(\frac{x}{\varepsilon}\right)\nabla u_2^\varepsilon\right) = -\frac{\kappa}{\varepsilon^2}\left(u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon\right) \\ \partial_t u_3^\varepsilon - \operatorname{div}\left(d_3(x)\mathbf{D}\left(\frac{x}{\varepsilon}\right)\nabla u_3^\varepsilon\right) = \frac{\kappa}{\varepsilon^2}\left(u_1^\varepsilon u_2^\varepsilon - \gamma u_3^\varepsilon\right) \end{cases}$$

♣ Supplement with

- initial data
- zero Neumann boundary condition

ENTROPY DISSIPATION STRUCTURE

- Multiply rate functions by logarithms: for $i = 1, 2,$

$$\mathcal{R}_i(u) = -\kappa\big(u_1 u_2 - \gamma u_3\big) \times \log(u_i)$$

$$\text{and} \qquad \mathcal{R}_3(u) = \kappa\big(u_1 u_2 - \gamma u_3\big) \times \log(\gamma u_3)$$

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- Summing the expressions

$$\mathcal{R}_1(u)\log(u_1) + \mathcal{R}_2(u)\log(u_2) + \mathcal{R}_3(u)\log(\gamma u_3)$$
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- Using logarithmic multipliers, the entropy dissipation inequality:

$$\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=1}^{3}\big(u_i\log(u_i) - u_i + c\big) \leq 0$$

STRATEGY FOR HOMOGENIZATION

♣ The evolution equation:

$$\partial_t u_i^\varepsilon - \operatorname{div}\left(d_i(x)\mathbf{D}\left(\frac{x}{\varepsilon}\right)\nabla u_i^\varepsilon\right) = \frac{1}{\varepsilon^2}\mathcal{R}_i(u^\varepsilon) \qquad \text{in } \Omega_T := (0,T)\times\Omega.$$

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♣ A typical homogenization result: for $\varepsilon \ll 1$,

$$u_i^\varepsilon(t,x) \approx u_i^*(t,x) + \varepsilon\, \widetilde{u}_i\left(t, x, \frac{x}{\varepsilon}\right)$$

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Find **uniform** bounds on $u_i^\varepsilon(t,x)$ in $\mathrm{L}^p\left((0,T);\mathrm{W}^{1,p}(\Omega)\right)$ for some $p>1$	$u_i^\varepsilon(t,x)$ relatively compact in $\mathrm{L}^p(\Omega_T)$ for some $p>1$
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$u_i^\varepsilon \rightharpoonup u_i^*$ in $\mathrm{L}^p\left((0,T);\mathrm{W}^{1,p}(\Omega)\right)$	i.e. $\Vert u_i^\varepsilon - u_i^*\Vert_{\mathrm{L}^p(\Omega_T)} \to 0$

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Step 4	Entropy inequality + Energy estimate $\Longrightarrow u_i^\varepsilon \in \mathrm{L}^{\frac{4}{3}}\left((0,T); \mathrm{W}^{1,\frac{4}{3}}(\Omega) \right)$

BATTLE PLAN II

Step 1	$u_1^\xi + u_3^\xi$ and $u_2^\xi + u_3^\xi$ are relatively compact in $\mathrm{L}^{\frac{4}{3}}(\Omega_T)$

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- ♣ Substitute algebraic relation to yield cross-diffusion interpretation.

BATTLE PLAN I – STEP 1

battle plan I – step 1

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Suppose the initial data $u_i^{\text{in}} \geq 0$.

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BATTLE PLAN I – STEP 2

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- Integrating above expression over $(0,T)$ yields the result.

BATTLE PLAN I – STEP 3

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The solution $u_i^\varepsilon(t,x)$ *satisfies*

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$$\Big(u_1^\varepsilon(t,x) + u_3^\varepsilon(t,x)\Big) - \mathrm{div}\left(\mathbf{D}\int_0^t \big(d_1\nabla u_1^\varepsilon(s,x) + d_3\nabla u_3^\varepsilon(s,x)\big)\mathrm{d}s\right) = \Big(u_1^{\mathrm{in}}(x) + u_3^{\mathrm{in}}(x)\Big)$$

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- Multiply by $\Big(d_1 u_1^\varepsilon + d_3 u_3^\varepsilon\Big)$ and some algebra yields result.

BATTLE PLAN I – STEP 4

Proposition (Weak compactness)

The solution $u_i^\varepsilon(t,x)$ *satisfies*

$$\|u_i^\varepsilon\|_{\mathrm{L}^{\frac{4}{3}}\left((0,T);\mathrm{W}^{1,\frac{4}{3}}(\Omega)\right)} \leq C.$$

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$$\left.\begin{aligned} \left\|\nabla\sqrt{u_i^\varepsilon}\right\|_{L^2(\Omega_T)} &\le C \\ \|u_i^\varepsilon\|_{L^2(\Omega_T)} &\le C \end{aligned}\right\} \implies \|\nabla u_i^\varepsilon\|_{L^{\frac{4}{3}}(\Omega_T)} \le C.$$

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- ♣ Using $\frac{3}{2}$ and 3 as Hölder conjugates, we have

$$\iint_{\Omega_T} |\nabla u_i^\varepsilon|^{\frac{4}{3}} = \iint_{\Omega_T} \frac{|\nabla u_i^\varepsilon|^{\frac{4}{3}}}{|u_i^\varepsilon|^{\frac{2}{3}}} |u_i^\varepsilon|^{\frac{2}{3}} \le \left(\iint_{\Omega_T} \left(\frac{|\nabla u_i^\varepsilon|^{\frac{4}{3}}}{|u_i^\varepsilon|^{\frac{2}{3}}} \right)^{\frac{3}{2}} \right)^{\frac{2}{3}} \left(\iint_{\Omega_T} \left(|u_i^\varepsilon|^{\frac{2}{3}} \right)^3 \right)^{\frac{1}{3}}$$

BATTLE PLAN II – STEP 1

Proposition (Relative compactness of sums)

The families $u_1^\varepsilon + u_3^\varepsilon$ *and* $u_2^\varepsilon + u_3^\varepsilon$ *are relatively compact in* $\mathrm{L}^{\frac{4}{3}}(\Omega_T)$.

Aubin-Lions compactness criterion

Let B_1, B_2, B_3 be Banach spaces such that $B_1 \subseteq B_2 \subseteq B_3$.
Suppose $w^\varepsilon \in \mathrm{L}^p((0,T); B_1)$ and $\partial_t w^\varepsilon \in \mathrm{L}^q((0,T); B_3)$ with $\frac{1}{p} + \frac{1}{q} = 1$.
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- Result follows by Aubin-Lions (take $p=\frac{4}{3}$ and $q=4$).

BATTLE PLAN II – STEP 2

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- Furthermore we have

$$0 \le u_1^\varepsilon \le u_1^\varepsilon + u_3^\varepsilon \to \mathrm{S}_{13} \quad \text{strongly in } \mathrm{L}^{\frac{4}{3}}(\Omega_T).$$

- Lebesgue's dominated convergence theorem then yields the result.

BATTLE PLAN II – STEP 3

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Proposition (Higher integrability)

The solution $u_i^\varepsilon(t,x)$ satisfies

$$\|u_i^\varepsilon\|_{\mathrm{L}^{4+\delta}(\Omega_T)} \le C \qquad \textit{for some } \delta > 0.$$

BATTLE PLAN II – STEP 3

♣ Consider the forward and backward heat equations

$$\begin{cases} \partial_t w - \Delta(\mu w) = 0 & \text{in } \Omega_T \\ w(0,x) = w^{\text{in}} & \text{in } \Omega \\ \nabla w \cdot \mathbf{n}(x) = 0 & \text{on } \partial\Omega_T \end{cases}$$

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Proposition (Parabolic duality estimates)

♣ Consider the forward and backward heat equations

$$\begin{cases} \partial_t w - \Delta(\mu w) = 0 & \text{in } \Omega_T \\ w(0,x) = w^{\text{in}} & \text{in } \Omega \\ \nabla w \cdot \mathbf{n}(x) = 0 & \text{on } \partial\Omega_T \end{cases} \qquad \begin{cases} \partial_t v + \mu \Delta v = \Theta & \text{in } \Omega_T \\ v(T,x) = 0 & \text{in } \Omega \\ \nabla v \cdot \mathbf{n}(x) = 0 & \text{on } \partial\Omega_T \end{cases}$$

where $0 < a \le \mu(t,x) \le b < \infty$.

Proposition (Parabolic duality estimates)

Given $\Theta \in \mathrm{L}^q(\Omega_T)$ *for some* $q \in (1,2]$, *we have*

$$\sup_{t\in[0,T]} \|v(t,\cdot)\|_{\mathrm{L}^q(\Omega)} \le C \|\Theta\|_{\mathrm{L}^q(\Omega_T)}$$

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Given $w^{\text{in}} \in \mathrm{L}^p(\Omega_T)$ *for some* $p \in [2,\infty)$, *we have*

$$\|w\|_{\mathrm{L}^p(\Omega_T)} \le C\,\left\|w^{\text{in}}\right\|_{\mathrm{L}^p(\Omega)}$$

BATTLE PLAN II – STEP 3

Proposition (Higher integrability)

The solution $u_i^\varepsilon(t,x)$ *satisfies*

$$\|u_i^\varepsilon\|_{\mathrm{L}^{4+\delta}(\Omega_T)} \leq C \qquad \textit{for some } \delta > 0.$$

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$$\partial_t \left(u_1^\varepsilon + u_3^\varepsilon\right) - d_1 \Delta u_1^\varepsilon - d_3 \Delta u_3^\varepsilon = 0$$

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$$\partial_t \left(u_1^\varepsilon + u_3^\varepsilon\right) - \Delta \left(\frac{d_1 u_1^\varepsilon + d_3 u_3^\varepsilon}{u_1^\varepsilon + u_3^\varepsilon} \left(u_1^\varepsilon + u_3^\varepsilon\right) \right) = 0.$$

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- Take

$$w(t,x) := u_1^\varepsilon + u_3^\varepsilon, \quad \mu(t,x) := \frac{d_1 u_1^\varepsilon + d_3 u_3^\varepsilon}{u_1^\varepsilon + u_3^\varepsilon}$$

- Parabolic duality estimates will yield the result.

BATTLE PLAN II – STEP 4

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Proposition (Relative compactness)

The solution families $u_i^\varepsilon(t,x)$ *are relatively compact in* $\mathrm{L}^4(\Omega_T)$.

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♣ Using interpolation in L^p-spaces yields

$$\left.\begin{aligned} \lim_{\varepsilon\to 0} \|u_i^\varepsilon - u_i^*\|_{\mathrm{L}^{\frac{4}{3}}(\Omega_T)} = 0 \\ \|u_i^\varepsilon\|_{\mathrm{L}^{4+\delta}(\Omega_T)} \le C \end{aligned}\right\} \implies \lim_{\varepsilon\to 0} \|u_i^\varepsilon - u_i^*\|_{\mathrm{L}^4(\Omega_T)} = 0.$$

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THANK YOU